Contents

Preface vii

Conference Organization viii

Word of Welcome ix

Yamada Science Foundation x

Executive Members of the Foundation xi

STM

Probing and inducing surface chemistry with the STM: the reactions of Si(111)-7 × 7 with H_2O and O_2
Ph. Avouris and I.-W. Lyo 1

Effect of tip atomic and electronic structure on scanning tunneling microscopy/spectroscopy
M. Tsukada, K. Kobayashi and N. Isshiki 12

The surface structure of an organic conductor $(BEDT\text{-}TTF)_2KHg(SCN)_4$ observed by scanning tunneling microscopy
M. Yoshimura, N. Ara, M. Kageshima, R. Shiota, A. Kawazu, H. Shigekawa, Y. Saito, M. Oshima, H. Mori, H. Yamochi and G. Saito 18

STRUCTURE

Surface step configurations under strain: kinetics and step–step interactions
M.B. Webb, F.K. Men, B.S. Schwartzentruber, R. Kariotis and M.G. Lagally 23

Rearrangement of surface steps of the Ni(7 9 11) surface by hydrogen adsorption
H. Namba, Y. Okawa and H. Kuroda 32

Structure of the K adsorbed Si(001)2 × 1 surface studied by LEED
T. Urano, Y. Uchida, S. Hongo and T. Kanaji 39

LEED and spectroscopic studies of (001) surfaces of Nd_2CuO_4 and $(NdCe)_2CuO_4$ single crystals
A.A. Abramov, N.V. Abrosimov, V.A. Grazhulis, A.M. Ionov and A.M. Panchenko 45

LEED-AES observations of the vacuum-cleaved Bi–Sr–Ca–Cu–O single crystals
H. Tokutaka, S. Kishida, H. Fujimoto, K. Nishimori and N. Ishihara 50

A study of the Si(111)$\sqrt{3} \times \sqrt{3}$-Ag surface by transmission X-ray diffraction and X-ray diffraction topography
T. Takahashi, S. Nakatani, N. Okamoto, T. Ishikawa and S. Kikuta 54

Surface structure of Cl/Ni(111) determined by surface EXAFS spectroscopy and soft X-ray standing-wave method
M. Funabashi, T. Yokoyama, Y. Takata, T. Ohta, Y. Kitajima and H. Kuroda 59

RHEED intensity analysis of Si(001)2 × 1 and 2 × 1-K surface structures
T. Makita, S. Kohmoto and A. Ichimiya 65

The direct observation of the Ge(001) dimer structure by high resolution UHV transmission electron microscopy
M. Mitome and K. Takayanagi 69

Short range orders of an adsorbed layer: gold on the Si(111)7 × 7 surface
S. Takahashi, Y. Tanishiro and K. Takayanagi 73

REM and TEM studies of 2D Au–Cu alloy adsorbates on a Si(111) surface
I. Homma, Y. Tanishiro and K. Yagi 81

TOF–ICISS study of surface damage formed by Ar ion bombardment of Si(100)
K. Sumitomo, K.-I. Tanaka, I. Katayama, F. Shoji and K. Oura 90

Characterization of organic ultra-thin films by Penning ionization electron spectroscopy during layer-by-layer preparation: TFTCNQ, TMTSF and their charge transfer complex
Y. Harada, H. Hayashi, S. Masuda, T. Fukuda, N. Sato, S. Kato, K. Kobayashi, H. Kuroda and H. Ozaki 95

PHASE TRANSITIONS

Lattice gas model of Si(111) and Ge(111)
J. Kanamori and Y. Sakamoto 102

Phase diagram of coadsorbate systems on the square lattice net
M. Kaburagi, T. Tonegawa and K. Ebina 107

Order–disorder transitions in fcc binary alloys with surfaces
Y. Teraoka 113

The (1×1) high temperature phase of Ge(111) and Si(111)
Y. Sakamoto and J. Kanamori 119

Three-body interaction between adsorbates
K. Ebina and M. Kaburagi 124

LEED observation of NO adsorption-induced relaxation on a single-domain Pt(001)–(20×5) surface
K. Mase and Y. Murata 132

Study of successive phase transitions of the Si(001)-Bi surface by RHEED
T. Hanada and M. Kawai 137

CRYSTAL GROWTH

Monte Carlo simulation of single domain Si(100) surfaces
T. Kawamura and P.A. Maksym 143

Periodic changes in the structure of a surface growing under MBE conditions and RHEED oscillation
T. Irisawa, A. Ichimiya and T. Kuroda 148

Hydrogen-termination effects on the growth of Ag thin films on Si(111) surfaces
M. Naitoh, F. Shoji and K. Oura 152

A RHEED study of the initial growth of Ag on the Si(001) surface
K. Nishimori, H. Tokutaka, T. Tamon, S. Kishida and N. Ishihara 157

Metastable structure of Si(111) surface during homoepitaxial growth
H. Nakahara and A. Ichimiya 162

Structure of GaAs heteroepitaxial layer grown on GaP(001) by molecular beam epitaxy
T. Nomura, K. Murakami, K. Ishikawa, M. Miyao, T. Yamaguchi, A. Sasaki and M. Hagino 166

ELECTROMIGRATION

Hetero-electromigration on semiconductor surfaces
H. Yasunaga 171

Surface electromigration of In and Cu on Si(111) surfaces studied by REM
A. Yamanaka and K. Yagi 181

Mass transport of a Ag thin film on a stepped Si(111) surface
N.-J. Wu, A. Natori and H. Yasunaga 191

Structural change of a heterogeneous thin film patch by surface electro-migration
A. Natori, S. Ohta and H. Yasunaga 195

PHYSISORBED LAYER

Calorimetric studies of phase transitions in submonolayer physisorbed phases
A. Inaba, T. Shirakami and H. Chihara 202

Magnetic phase transition in adsorbed ^{3}He films
K. Machida 206

Magnetic phase transition of oxygen monolayer films adsorbed on exfoliated graphite
Y. Murakami and H. Suematsu 211

ELECTRONIC STRUCTURE (THEORY)

Theory of surface stress and surface reconstruction
R.J. Needs, M.J. Godfrey and M. Mansfield 215

Self-consistent calculation of the bandgap and screening at Si(111)2×1
L. Reining and R. Del Sole 222

Electronic structure of the DAS model for the Si(111)7×7 reconstructed surface by energy band calculations
M. Fujita, H. Nagayoshi and A. Yoshimori 229

Electronic states of Si(001) stepped surfaces
T. Yamaguchi and N. Fujima 233

Electronic structure of the Si(111)$\sqrt{3} \times \sqrt{3}$ surface with column V adatoms
H. Nagayoshi 239

UPS, PED, IPS, AND OTHERS

The extra branch of ARUPS spectra and the atomic structure of the Si(100) surface
K. Inoue, M. Nakayama and H. Kawai 244

Theoretical analysis of angle-resolved photoemission for simple metals
A. Ishii and T. Aisaka 250

Surface electronic structure determination by positronium formation spectroscopy
A. Ishii and S. Shindo 256

Photoemission from the 2p core of surface dimers on Si(100)
T. Yamazaki and K. Cho 260

Theory of resonant photoemission of adsorbates on metal surfaces
H. Ueba 266

Angle-resolved photoemission studies of clean and adsorbed Si(001) surfaces: 2×1, c(4×2), 2×1–Na and 2×2–Ga
Y. Enta, S. Suzuki and S. Kono 277

Existence of Ga dangling bonds on As-stabilized GaAs(100)(2×4)–c(2×8) and $Al_xGa_{1-x}As$(100) surfaces
X.M. Ding, T. Miyahara, H. Okumura, S. Muto, H. Namba and H. Kuroda 284

Two-dimensional photoelectron diffraction patterns by display-type spherical mirror analyzer
H. Daimon, Y. Tezuka, A. Otaka, N. Kanada, S.K. Lee, S. Ino, H. Namba and H. Kuroda 288

Inverse photoemission study of transition metal intercalation and surface adsorbed TiS_2
H. Namatame, S. Nohara, H. Negishi, M. Inoue and S. Suga 294

Theory of nonlinear surface magneto-optics: inclusion of band structure and matrix elements for ferromagnetic nickel
W. Hübner and K.-H. Bennemann 299

Role of surface electronic transitions in linear and nonlinear electromagnetic phenomena at noble metal surfaces: beyond jellium
M.Y. Jiang, G. Pajer and E. Burstein 306

INTERFACES

Hydrogen-induced surface acceptors on GaAs(110) surfaces at low temperatures
T.U. Kampen, L. Koenders, K. Smit, M. Rückschloss and W. Mönch 314

The influence of a RbF interlayer on the Ge/GaAs interface properties
R. Klauser, M. Oshima, H. Sugahara and Y. Murata 319

Nitride layers on GaAs(110) surfaces
D. Troost, H.-U. Baier, A. Berger and W. Mönch 324

Nonmetal to metal phase transition in the Mn/Si(111)7 × 7 system
S. Kawamoto, M. Kusaka, M. Hirai and M. Iwami 331

Bonding states of chemisorbed sulfur atoms on GaAs
H. Sugahara, M. Oshima, R. Klauser, H. Oigawa and Y. Nannichi 335

ALKALI-METAL ADSORPTION

Theory of alkali adsorption on simple metal surfaces
H. Ishida 341

Atomic arrangement of alkali adatoms on the Si(001)–2 × 1 surface
K. Kobayashi, S. Blügel, H. Ishida and K. Terakura 349

Peierls instability considerations for alkali metal chains on Si(001)-2 × 1
I.P. Batra 354

Charge transfer and promoted oxygen uptake at alkalated Si(100) surfaces studied by Auger deexcitation of helium metastables
S. Nishigaki, T. Sasaki, S. Matsuda, N. Kawanishi, H. Takeda and K. Yamada 358

BEAM STUDIES

Aspects of molecule–surface interactions
B.I. Lundqvist 365

Classical trajectory study of the interaction of oriented NO and Ag(111)
M.G. Tenner, E.W. Kuipers, A.W. Kleyn and S. Stolte 376

Molecular beam study on scattering and sticking of molecular oxygen at Si(100)
T. Miyake, S. Soeki, H. Kato, T. Nakamura, A. Namiki, H. Kamba and T. Suzaki 386

Vibrational excitation dynamics in molecule–surface scattering
H. Kasai and A. Okiji 394

Two-hole states of the outermost surface layer studied by metastable atom electron spectroscopy. Si(111)–7 × 7 and Si(100)–2 × 1
S. Masuda, H. Ishii and Y. Harada 400

Separation of scattered ions and neutrals in CAICISS with an acceleration tube
I. Kamiya, M. Katayama, E.Nomura and M. Aono 404

Electron correlation effects on charge transfer and energy dissipation in atom or ion scattering from metal surfaces
H. Nakanishi, H. Kasai and A. Okiji 410

Secondary electron spectra from a tantalum surface by multiply charged ions
T. Kanie, K. Oda, A. Ichimiya, T. Yasue, S. Ohtani and H. Tawara 417

Low-energy recoil-ion spectroscopy studies of hydrogen adsorption on Si(100)–2 × 1 surfaces
F. Shoji, K. Kashihara, K. Sumitomo and K. Oura 422

A study of matrix effects in CsI on Au by time-of-flight SIMS
Y.S. Kim, D.W. Moon, J.C. Lee and H.J. Kang 428

On the radial distribution function for sub-kV backscattered electron diffraction from a disordered surface
H. Yoshikawa, Z.-J. Ding and R. Shimizu 434

DESORPTION

Two dimensional imaging of photodesorbed species from surfaces and the desorption dynamics
R. Schwarzwald, A. Mödl and T.J. Chuang 437

Photostimulated desorption of NO on Pt(001) studied with a multiphonon ionization technique
K. Mase, S. Mizuno, Y. Achiba and Y. Murata 444

A study of the oxygen adsorption process on a titanium single crystal surface by electron stimulated desorption
A. Takano and K. Ueda 450

A study of hydrogen adsorption on the silicon single crystal surfaces by electron stimulated desorption (TOF-ESD)
K. Ueda, S. Kodama and A. Takano 454

Formation and desorption of aluminum hydride from hydrogen adsorbed aluminum surfaces
M. Hara, K. Domen, T. Onishi, H. Nozoye, C. Nishihara, Y. Kaise and H. Shindo 459

Thermal desorption of molecules coadsorbed on metal surfaces
M. Mizuno, H. Kasai and A. Okiji 464

REACTIONS, REACTIVE SURFACES

Molecule–surface complexes and catalytic reactions
E. Ilisca 470

Silicon precipitation in a surface layer of SiO_2 by high-power vacuum ultraviolet laser irradiation
K. Kurosawa, Y. Takigawa, W. Sasaki, M. Okuda and Y. Inoue 475

The puzzles of surface science and recent attempts to explain them
G.A. Somorjai 481

Spatial distribution of reactive CO_2 desorption on Pt(110)(1 × 2) surfaces
T. Matsushima 489

Chemisorption and thermal decomposition of ethylene on clean and modified Pd(110) surfaces: electron energy loss spectroscopy, low-energy electron diffraction, and thermal desorption studies
M. Nishijima, T. Sekitani, J. Yoshinobu and M. Onchi 493

Chemical reactivity of the Si(100)(2 × 1)-K surface: electron energy loss spectroscopy and thermal desorption studies
M. Nishijima, S. Tanaka, N. Takagi and M. Onchi 498

Synthesis of metastable surface complexes by chemical reactions. N and NH_x complexes on Pd(100), Rh(100) and Pt–Rh(100)
K.-I. Tanaka, T. Yamada and B.E. Nieuwenhuys 503

The reaction of copper and calcium dipivaloylmethanates ($Cu(DPM)_2$ and $Ca(DPM)_2$) with hydroxyls on oxide surface
R. Sekine, M. Kawai, T. Hikita and T. Hanada 508

Oxygen isotope exchange between O_2 adsorbate and UV-irradiated MgO surfaces
Y. Yanagisawa, R. Huzimura, K. Matsumura and S. Yamabe 513

PHONONS, VIBRATIONS

One-phonon and multiphonon processes in atom–surface scattering
V. Celli, D. Himes, V. Bortolani, G. Santoro, J.P. Toennies and G. Zhang 518

Vibrational dynamics of the ideally H-terminated Si(111) surface
Y.J. Chabal, P. Dumas, P. Guyot-Sionnest and G.S. Higashi 524

A molecular orbital study for CO coadsorbed with K on Cu(001) and Ag(001)
E. Miyoshi, Y. Sakai and S. Katsuki 531

Infrared spectra of CO adsorbed on Pt(100), Pt(111), and Pt(110) electrode surfaces
Y. Kinomoto, S. Watanabe, M. Takahashi and M. Ito 538

Absolute Raman scattering cross sections of surface adsorbed Cu–phthalocyanine molecules
M. Kuwahara, G. Mizutani, K. Sakamoto and S. Ushioda 544

Raman study of a silver electrode in electrolytes with SO_4^{2-} ions
Y. Sasaki and Y. Nishina 549

Author index 554

Subject index 560